

Positive semidefinite rank and nested spectrahedra

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Abstract

The set of matrices of given positive semidefinite rank is semialgebraic. In this paper we study its geometry and in small cases we describe its boundary. For general psd rank we give a conjecture for its boundary and for its semialgebraic description. Our proof techniques are based on studying nested spectrahedra and spectrahedral shadows.

1 Introduction

Standard matrix factorization is used in a wide range of applications in statistics, optimization, machine learning, and many others. Given a matrix $M \in \mathbb{R}^{p \times q}$ of rank k , the goal is to find vectors $a_1, \dots, a_p, b_1, \dots, b_q \in \mathbb{R}^k$ such that the i, j -th entry of M is $M_{ij} = \langle a_i, b_j \rangle$.

Often times, however, applications impose further conditions on the factors a_i and b_j . This is why recent studies [3, 5, 6] have addressed the notion of *conic matrix factorization* in which $M_{ij} = \langle a_i, b_j \rangle$ and the elements $a_1, \dots, a_p, b_1, \dots, b_q$ are required to lie in a given cone K (or its dual K^*). For example, when K is the nonnegative orthant $\mathbb{R}_{\geq 0}^k$, one obtains nonnegative matrix factorization [1, 4, 12, 18]. In this article we focus on the case when K is the cone of $k \times k$ symmetric positive semidefinite matrices \mathcal{S}_+^k , which lies inside the space of $k \times k$ symmetric matrices \mathcal{S}^k equipped with the trace inner product

$$\langle A, B \rangle = \text{trace}(A, B).$$

Definition 1.1. *Given a nonnegative matrix $M \in \mathbb{R}^{p \times q}$, a positive semidefinite (psd) factorization of size k is a collection of matrices $A_1, \dots, A_p, B_1, \dots, B_q \in \mathcal{S}_+^k$ such that $M_{ij} = \langle A_i, B_j \rangle$. The positive semidefinite rank (or psd rank) of the matrix M is the smallest number k for which such a factorization exists. It is denoted by $\text{rank}_{\text{psd}}(M)$.*

The geometric aspects of positive semidefinite rank have been studied in a number of recent articles [2, 5, 6, 7, 8, 9].

Let $\mathcal{M}_{r,k}^{p \times q}$ (for short $\mathcal{M}_{r,k}$ if p and q are understood from the context) denote the set of $p \times q$ nonnegative real matrices of rank at most r and psd rank at most k . By Tarski-Seidenberg's Theorem this set is semialgebraic, i.e. it is defined by a finite set of unions,

intersections and complements of polynomial equalities and inequalities. It lies inside the space of $p \times q$ matrices of rank at most r , denoted by $\mathcal{V}_r^{p \times q}$ (for short \mathcal{V}_r). In this article, we study the geometry of $\mathcal{M}_{r,k}$. For small values of r and k , we describe its *topological boundary* $\partial\mathcal{M}_{r,k}$, as well as its *algebraic boundary* $\overline{\partial\mathcal{M}_{r,k}}$. The topological boundary $\partial\mathcal{M}_{r,k}$ is the boundary of $\mathcal{M}_{r,k}$ as a subset of \mathcal{V}_r , and its algebraic boundary $\overline{\partial\mathcal{M}_{r,k}}$ is the Zariski closure of $\partial\mathcal{M}_{r,k}$.

Given a nonnegative matrix M of rank $n+1$, one can associate to M two nested polytopes $P \subseteq Q \subset \mathbb{R}^n$ (see Section 2). Theorem 2.1, proven in [9], shows that M has psd rank at most k if and only if one can fit a projection of a slice of the space of $k \times k$ positive semidefinite matrices S_+^k between P and Q . This geometric interpretation is analogous to the result of Cohen and Rothblum in [1] for nonnegative matrix factorization in which case one needs to nest a polytope between P and Q .

In this article we focus on describing $\partial\mathcal{M}_{k+1,k}$, in other words we restrict to the case when $\text{rank}(M) = \text{rank}_{\text{psd}}(M) + 1$. In Section 3, we consider $k = 2$. Geometrically, a matrix M has rank 3 and psd rank 2 if and only if one can fit an ellipse between the two nested polygons $P \subseteq Q \subset \mathbb{R}^2$ associated to M . In Theorem 3.2, we show that M lies on the boundary $\partial\mathcal{M}_{3,2}$ if and only if every ellipse that fits between P and Q goes through at least three of the vertices of P and touches at least three of the sides of Q .

In Conjecture 4.1 we generalize Theorem 3.2 for psd rank k and rank $k+1$. Section 4 is devoted to giving a geometric interpretation of this conjecture and Section 5 provides strong geometric and computational evidence towards proving it. For instance, in Lemma 5.1 we show that one can consider nesting spectrahedra instead of nesting general spectrahedral shadows. In Section 5.2 we give computational evidence towards Conjecture 4.1 and state some open questions. The code for our computations is available at

<https://github.com/kaiekubjas/psd-rank>

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2 Preliminaries

Many of the basic results related to psd rank have been studied in [2]. We give a brief overview of the results we use throughout the article.

2.1 Bounds

The positive semidefinite rank of a matrix is bounded below by the inequality

$$\text{rank}(M) \leq \binom{\text{rank}_{\text{psd}}(M) + 1}{2}$$

since one can vectorize the symmetric matrices in a given psd factorization and consider the trace inner product as a dot product. On the other hand, the psd rank is upper bounded by the nonnegative rank

$$\text{rank}_{\text{psd}}(M) \leq \text{rank}_+(M)$$

since one can obtain a psd factorization from a nonnegative factorization by using diagonal matrices. The psd rank of M can be any integer satisfying these inequalities.

2.2 Geometric description

We now describe the geometric interpretation of psd rank. Let $P \subseteq \mathbb{R}^n$ be a polytope and $Q \subseteq \mathbb{R}^n$ be a polyhedron such that $P \subseteq Q$. Assume that P is the convex hull of p points: $P = \text{conv}\{v_1, \dots, v_p\}$ and Q has the following representation in terms of its facets: $Q = \{x \in \mathbb{R}^n | h_j^T x \leq 1, j = 1, \dots, q\}$, where $v_1, \dots, v_p, h_1, \dots, h_q \in \mathbb{R}^n$. Then, the *slack matrix* of the pair P, Q , denoted $S_{P,Q}$ is the $p \times q$ matrix whose i, j -th entry is $1 - h_j^T v_i$. When $P = Q$ then $S_P := S_{P,P}$ is the *slack matrix* of P .

Conversely, suppose we start with a nonnegative matrix M of rank $n + 1 \leq \min\{p, q\}$ and suppose that the vector $\mathbf{1} := (1 \ \cdots \ 1)$ lies in the column and the row span of M . Consider *any* factorization $M = CD$, where $C \in \mathbb{R}^{p \times (n+1)}$ and $D \in \mathbb{R}^{(n+1) \times q}$ are matrices with real entries and the last column of C is $\mathbf{1}$ and the last row of D is $\mathbf{1}$. Let $(c_1, 1), \dots, (c_p, 1)$ be the rows of C and $(-d_1, 1), \dots, (-d_q, 1)$ be the columns of D . Then, $M_{i,j} = 1 - \langle c_i, d_j \rangle$ and since M is nonnegative, $\langle c_i, d_j \rangle \leq 1$ for all i, j . Then, M is the slack matrix of the polytope $P = \text{conv}\{c_1, \dots, c_p\}$ whose vertices are the points c_1, \dots, c_p and the polyhedron $Q = \{x \in \mathbb{R}^n | \langle d_j, x \rangle \leq 1\}$. So, $M = S_{P,Q}$.

Theorem 2.1 (Proposition 3.6 in [9]). *Let $P \subset \mathbb{R}^n$ be a polytope and $Q \subseteq \mathbb{R}^n$ a polyhedron such that $P \subseteq Q$. Then, $\text{rank}_{\text{psd}}(S_{P,Q})$ is the smallest integer k for which there exists an affine subspace \mathcal{L} of \mathcal{S}^k and a linear map π such that $P \subseteq \pi(\mathcal{L} \cap \mathcal{S}_+^k) \subseteq Q$.*

In other words, the matrix $S_{P,Q}$ has psd rank at most k if and only if one could fit a linear image of a spectrahedron of size k between P and Q .

Remark 2.2. *Note that given M the polytopes P and Q are not unique. Moreover, given P and Q , the slack matrix of P and Q depends on the choice of inequality description of Q . However, as Theorem 2.1 suggests, the psd factorization properties are preserved regardless of the choices one makes.*

Now consider a matrix $M \in \mathbb{R}_{\geq 0}^{m \times n}$ of rank 3. It has a factorization $M_{ij} = \langle u_i, v_j \rangle$, where $u_i, v_j \in \mathbb{R}^3$. Thus, we get two nested polygons $P \subseteq Q \subset \mathbb{P}^2$, where $P = \text{conv}(u_1, \dots, u_m) \subset \mathbb{P}^2$ and $Q = \{x \in \mathbb{P}^2 : x^T V \geq 0\}$. Moreover, the matrix M has psd rank 2 if and only if we can fit an ellipse between the two polygons P and Q [9, Proposition 4.1].

3 Rank 3 and psd rank 2

The aim of this section is to study the topological and algebraic boundaries of $\mathcal{M}_{3,2}^{p \times q}$. First, we make the following observation.

Proposition 3.1. *The Zariski closure of $\mathcal{M}_{3,2}^{p \times q}$ is $\mathcal{V}_3^{p \times q}$.*

Proof. Consider a matrix $M \in \mathcal{M}_{3,2}^{p \times q}$ such that the polygon P is very small relative to Q . If we change M continuously without changing the rank, then the vertices and facets of P and Q change continuously as well, see proof of [12, Lemma 4.3]. Hence we will be able to fit an ellipse between the P' and Q' arising from any M' in a small neighborhood $B \cap \mathcal{V}_3^{p \times q}$ of M , and the dimension of $\mathcal{M}_{3,2}^{p \times q}$ is equal to that of $\mathcal{V}_3^{p \times q}$. Since $\mathcal{M}_{3,2}^{p \times q} \subset \mathcal{V}_3^{p \times q}$ and $\mathcal{V}_3^{p \times q}$ is irreducible, we must have the result. \square

The following theorem is the main result of this section.

Theorem 3.2. *We describe the topological and algebraic boundaries of $\mathcal{M}_{3,2}^{p \times q}$.*

- a. *A matrix $M \in \mathcal{M}_{3,2}^{p \times q}$ lies on the topological boundary $\partial \mathcal{M}_{3,2}^{p \times q}$ if and only if $M_{ij} = 0$ for some i, j , or each ellipse that fits between the two polygons P and Q contains at least 3 vertices of the inner polygon P and is tangent to at least 3 sides of the outer polygon Q .*
- b. *A matrix $M \in \overline{\mathcal{M}_{3,2}^{p \times q}} = \mathcal{V}_3$ lies on the algebraic boundary $\overline{\partial \mathcal{M}_{3,2}^{p \times q}}$ if and only if $M_{ij} = 0$ for some i, j or there exists an ellipse that contains at least three vertices of P and is tangent to at least three edges of Q .*
- c. *The algebraic boundary of $\mathcal{M}_{3,2}^{p \times q}$ is the union of $\binom{p}{3} \binom{q}{3} + pq$ irreducible components. Besides the mn components $M_{ij} = 0$, there are $\binom{p}{3} \binom{q}{3}$ components each of which is defined by the 4×4 minors of M and one additional polynomial equation with 1035 terms homogeneous of degree 24 in the entries of M and homogeneous of degree 8 in each row and each column of a 3×3 submatrix of M .*

Proof.

(a) Only if: We will show the contrapositive of the statement: If all entries of M are positive and there is an ellipse between P and Q that contains at most two vertices of P or is tangent to at most two edges of Q , then M lies in the interior of $\mathcal{M}_{3,2}^{p \times q}$.

First, if there is an ellipse E between P and Q that touches neither of the polytopes, then M is in the interior of $\mathcal{M}_{3,2}^{p \times q}$: The vertices and facets of P and Q change continuously if we keep the rank of M fixed, see proof of [12, Lemma 4.3]. It follows that for every M' in a small neighborhood of M , we can find an ellipse between P' and Q' .

If at most two edges of Q are tangent to an ellipse E , then $P \subset E \subset Q$ can be transformed such that the two tangent facets are $x = 0$ and $y = 0$ and that the points of tangency are $(0, 1)$ and $(1, 0)$. This can be achieved by choosing a projective transformation L such that active facets become $(0, 1, 0)^T$ and $(0, 0, 1)^T$ in $L^{-1}V$. We consider a family of ellipses of the form $\{(x, y) : x^2 + bxy + y^2 - 2x - 2y + 1 = 0\}$ for some b with $0 < b^2 < 4$. Given an ellipse in this family, we choose one with slightly smaller b to get a slightly larger ellipse E' with the same points of tangency. Since the original ellipse E without the tangency points is strictly contained in E' and P is contained in the interior of Q (since M is positive), then P is strictly contained in E' . Thus M lies in the interior of $\mathcal{M}_{3,2}^{p \times q}$. The case when E goes through at most two vertices of P follows by duality.

If: Again, we will show the contrapositive of the statement: If $M \in \mathcal{M}_{3,2}^{p \times q}$ lies in the interior, then there is an ellipse between P and Q that does not touch P .

Let M be a matrix in the interior of $\mathcal{M}_{3,2}^{p \times q}$. Then there exists an open ball \mathcal{B} around M such that every $M' \in \mathcal{B} \cap \mathcal{V}_3^{p \times q}$ is also contained in $\mathcal{M}_{3,2}^{p \times q}$. Now choose $M' \in \mathcal{B} \cap \mathcal{V}_3^{p \times q}$ such that the columns of M' are in $\text{span}(M)$ and $\text{cone}(M') = t \cdot \text{cone}(M)$ for some $t > 1$. We have $Q' = Q$ and P is contained in the interior of P' . Since $M' \in \mathcal{M}_{3,2}^{p \times q}$, there exists an ellipse E' that fits between P' and Q' . Therefore, E' fits between P and Q and it does not touch P .

(b), (c) Given three points a, b, c in \mathbb{P}^2 and three lines d, e, f in \mathbb{P}^2 , each given by three homogeneous coordinates, we seek the condition that there exists an ellipse X such that a, b, c lie on X and d, e, f are tangent to X .

Let $X = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{12} & x_{22} & x_{23} \\ x_{13} & x_{23} & x_{33} \end{bmatrix}$ be the matrix of an ellipse. Then the corresponding ellipse curve goes through the points a, b, c if and only if

$$a^T X a = b^T X b = c^T X c = 0. \quad (3.1)$$

Similarly, the lines d, e, f are tangent to the ellipse curve if and only

$$d^T Y d = e^T Y e = f^T Y f = 0, \quad (3.2)$$

where $XY = I_3$. We seek to eliminate the variables X and Y .

Let $[a, b, c]$ denote the matrix whose columns are a, b, c . First we assume that $[a, b, c]$ is the 3×3 -identity matrix. Then we proceed in two steps:

1) The equations (3.1) imply that x_{11}, x_{22}, x_{33} are zero. We make the corresponding replacements in equations (3.2).

2) We use [16, formula (4.5) on page 48] to get the resultant of three ternary quadrics to get a single polynomial in the entries of d, e, f .

Now we use representation theory to obtain the desired polynomial in the general case. Let $g \in \text{GL}_3(\mathbb{R})$. The ellipse X goes through the points a, b, c and touches the lines d, e, f if and only if the ellipse $g^{-T} X g^{-1}$ goes through the points ga, gb, gc and touches the lines $g^{-T}d, g^{-T}e, g^{-T}f$. Thus our desired polynomial belongs to the ring of invariants $\mathbb{R}[V^3 \oplus V^{*3}]^{\text{GL}_3(\mathbb{R})}$ where $V = \mathbb{R}^3$ and the action of $\text{GL}_3(\mathbb{R})$ on $V^3 \oplus V^{*3}$ is given by

$$g \cdot (a, b, c, d, e, f) := (ga, gb, gc, g^{-T}d, g^{-T}e, g^{-T}f).$$

The First Fundamental Theorem states that $\mathbb{R}[V^3 \oplus V^{*3}]^{\text{GL}_3(\mathbb{R})}$ is generated by the bilinear functions $(i|j)$ on $V^3 \oplus V^{*3}$ defined by

$$(i|j) : (a, b, c, d, e, f) \mapsto ([a, b, c]^T [d, e, f])_{ij}.$$

For the FFT see for example [11, Chapter 2.1]. In the special case when $[a, b, c]$ is the 3×3 identity matrix, $(i|j)$ maps to the (i, j) -th entry of $[d, e, f]$. Hence to obtain the desired polynomial in the general case, we replace in the resultant obtained in the special case the entries of the matrix $[d, e, f]$ by the entries of the matrix $[a, b, c]^T [d, e, f]$.

Maple code for doing the steps in the previous paragraphs can be found at our website. This program outputs one polynomial of degree 1035 homogeneous of degree 8 in each of

the rows and the columns of the matrix $\begin{bmatrix} - & a & - \\ - & b & - \\ - & c & - \end{bmatrix} \begin{bmatrix} | & | & | \\ d & e & f \\ | & | & | \end{bmatrix}$. By construction, if this homogeneous polynomial vanishes and the convex hull of a, b, c lies inside the triangle with sides d, e, f and a, b, c, d, e, f are real, then there exists an ellipse nested between the polytopes touching d, e, f and containing a, b, c . Therefore, the Zariski closure of the condition that the only possible ellipses that can fit between the two polygons touch at least 3 sides of the outer polygon and at least 3 vertices of the inner polygon is exactly that there exists an ellipse that touches at least 3 sides of the outer polygon and at least 3 vertices of the inner polygon. This proves (b).

To prove (c), let $M \in \mathcal{V}_3^{p \times q}$ be such that $M = UV$ and a, b, c are three of the rows of U and d, e, f are three of the columns of V . Then, the above-computed polynomial is in the entries of a 3×3 submatrix of M corresponding to these rows and columns. For each three rows of and three columns of M we have one such polynomial, so the algebraic boundary is given by the union over each 3 rows and 3 columns of M of the variety defined by the 4×4 minors of M and the corresponding degree 24 polynomial with 1035 terms. \square

We now investigate the topological boundary more thoroughly.

Proposition 3.3. *Suppose $M \in \mathcal{M}_{3,2}^{p \times q}$ is strictly positive. Then M lies on the topological boundary if and only if there exists a unique ellipse that nests between P and Q .*

Proof. A matrix in the relative interior of $\mathcal{M}_{3,2}^{p \times q}$ will have multiple ellipses nested between P and Q : If there exists some nested ellipse that does not intersect P , we can just take slight scalings of this ellipse. This proves the “if” direction.

For the “only if” direction, suppose M lies on the topological boundary and E_0 and E_1 are two ellipses nested between P and Q . Let $E_{1/2}$ be the ellipse determined by averaging the quadratics defining E_0 and E_1 , i.e.

$$E_{1/2} = \{x \mid q_0(x) + q_1(x) \geq 0\} \text{ where } E_i = \{x \mid q_i(x) \geq 0\}.$$

It is straightforward to see that $E_{1/2}$ is nested between P and Q . Furthermore, if v is a vertex of P , then $E_{1/2}$ passes through v if and only if both E_0 and E_1 pass through v . Similarly, if f is a facet of Q , then $E_{1/2}$ is incident to f if and only if E_0 and E_1 are tangent to f at the same point. By Theorem 3.2, the ellipse $E_{1/2}$ must pass through three vertices of P and three facets of Q . Hence, there must exist six distinct points that both E_0 and E_1 pass through. Since five distinct points determine a conic, we must have that $E_0 = E_1$. \square

Example 3.4. *In the previous result, we examined the geometric configurations on the boundary of the semialgebraic set coming from strictly positive matrices. The simplest idea for such a matrix is to take two equilateral triangles and expand the inner one until we are on a boundary configuration as in Figure 1a.*

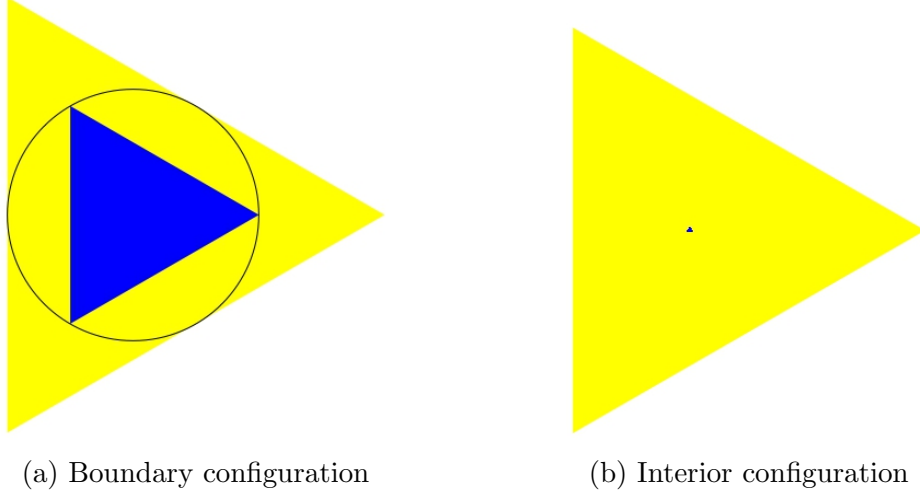


Figure 1: Geometric configurations of matrices in $\mathcal{M}_{3,2}^{3 \times 3}$

This configuration has the slack matrix

$$\begin{bmatrix} 4 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 4 \end{bmatrix}.$$

The 1035 term boundary polynomial from Theorem 3.2 vanishes on this matrix, as we expect.

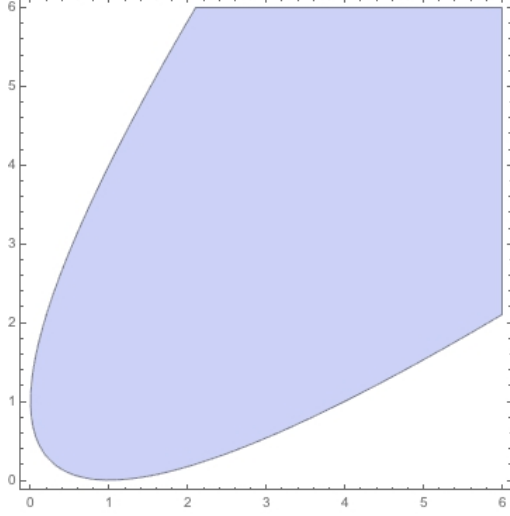
This matrix lies in the set of 3×3 circulant matrices which have the form

$$\begin{bmatrix} a & b & c \\ c & a & b \\ b & c & a \end{bmatrix}.$$

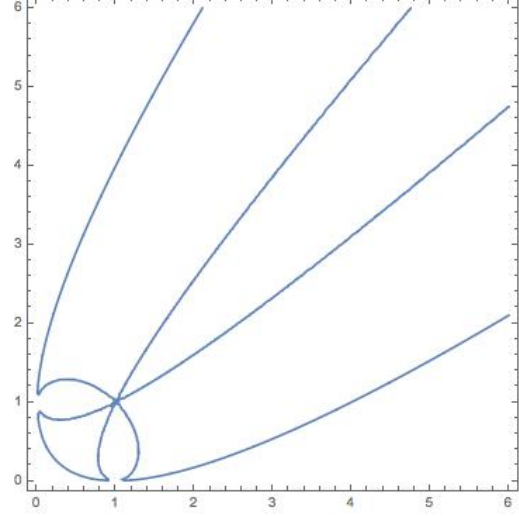
It was shown in [2, Example 2.7] that these matrices have psd rank at most two precisely when $a^2 + b^2 + c^2 - 2(ab + ac + bc) \leq 0$. As expected, whenever this polynomial vanishes, the 1035 term boundary polynomial vanishes as well. Figure 1b shows an instance of parameters a, b, c such that the matrix is on the algebraic boundary but not on the topological boundary – the polynomial vanishes, but the matrix lies in the interior of $\mathcal{M}_{3,2}$.

We were interested in finding out if the boundary polynomial could be used in an inequality to classify circulant matrices of psd rank at most two. However, as the contour plot in Figure 2b shows the circulant matrices of psd rank at most two in Figure 2a take both positive and negative values of the boundary polynomial. Figures 3a and 3b show the semialgebraic set and the boundary polynomial in the 3-dimensional space.

The phenomenon that the algebraic boundary of a semialgebraic set is relatively simple, e.g. consists of coordinate hyperplanes and one additional polynomial, but a semialgebraic description involves other polynomials also happens in the case of matrices of nonnegative rank at most three [12, Section 4] and partial matrices that can be completed to a rank one matrix in the standard simplex [13, Section 3].

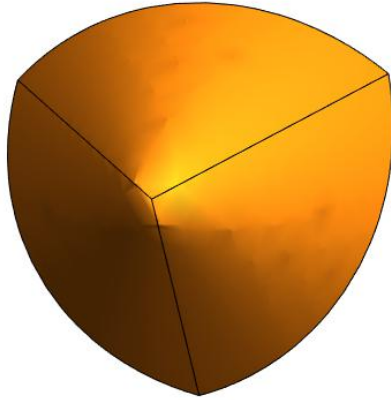


(a) Circulant matrices of psd rank at most 2

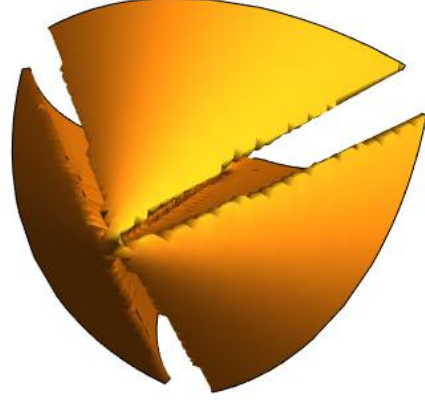


(b) The boundary polynomial

Figure 2: 3×3 circulant matrices in \mathbb{R}^2



(a) Circulant matrices of psd rank at most 2



(b) The boundary polynomial

Figure 3: 3×3 circulant matrices in \mathbb{R}^3

4 Geometric interpretation

In this section we generalize our results from the previous section to any psd rank k and we explain geometrically what it means for a matrix to lie on the boundary.

Conjecture 4.1. *A matrix $M \in \mathcal{M}_{k+1,k}^{p \times q}$ lies on the boundary $\partial \mathcal{M}_{k+1,k}^{p \times q}$ if and only if for every psd factorization $M_{ij} = \langle A_i, B_j \rangle$ with $A_i, B_j \in \mathcal{S}_+^k$, there exist $1 \leq i_1 < \dots < i_{k+1} \leq p$ and $1 \leq j_1 < \dots < j_{k+1} \leq q$ such that*

$$\text{rank}(A_{i_1}) = \dots = \text{rank}(A_{i_{k+1}}) = \text{rank}(B_{j_1}) = \dots = \text{rank}(B_{j_{k+1}}) = 1.$$

Our aim here is to give a geometric interpretation of this conjecture. Assume that $(1 \ \cdots \ 1)^T$ lies in both the column span and the row span of M . Let $M = VH$ be a rank $k + 1$ factorization of M such that

$$V = \begin{bmatrix} - & v_1 & - & 1 \\ - & v_2 & - & 1 \\ & \vdots & & \vdots \\ - & v_p & - & 1 \end{bmatrix} \quad \text{and} \quad H = \begin{bmatrix} | & | & & | \\ -h_1 & -h_2 & \cdots & -h_q \\ | & | & & | \\ 1 & 1 & \cdots & 1 \end{bmatrix}.$$

Consider the polytope P with vertices v_1, \dots, v_p and origin in its interior, and the polyhedron Q with facets $\langle h_i, x \rangle \leq 1$ for $i = 1, \dots, q$. Then, M is their slack matrix since the (i, j) -th entry of $M = 1 - \langle h_i, v_j \rangle$ is the dot product of the i -th row of V and the j -th column of H .

Let $A_1, \dots, A_p, B_1, \dots, B_q \in \mathcal{S}_+^k$ give a size k psd factorization of M . We define two S_+^k -lifts that are nested between P and Q as in [6, Section 4.1]:

$$\begin{aligned} C_A &= \{x \in \mathbb{R}^n : \exists y \in S_+^k \text{ s.t. } 1 - \langle h_i, x \rangle = \langle A_i, y \rangle \text{ for } i = 1, \dots, q\}, \\ C_B &= \{Vz : \mathbf{1}^T z = 1, Bz \in S_+^k\}. \end{aligned}$$

By [6, Proposition 4.1], we have

$$P \subseteq C_B \subseteq C_A \subseteq Q.$$

Since $1 - \langle h_i, v_j \rangle = \langle A_i, B_j \rangle$, the matrix B_j in the S_+^k -lift of C_A projects to $v_j \in C_A$. If $\text{rank}(B_j) = 1$, then v_j lies in the rank one locus of the spectrahedral shadow C_A .

In the dual picture, the inner polytope P becomes the outer polytope P° and the outer polytope Q becomes the inner polytope Q° . The vertices of Q° are given by h_1, \dots, h_q and the facets of P° are given by $\langle v_j, x \rangle \leq 1$ for $j = 1, \dots, p$.

Lemma 4.2. *The dual of the convex body C_A is the convex body $\{w^T H : w^T \mathbf{1} \leq 1, w^T A \in S_+^k\}$.*

Proof. This proof is very similar to the proof of [6, Theorem 2.7]. By definition

$$(C_A)^\circ = \{z \in \mathbb{R}^n : z^T x \leq 1 \ \forall x \in C_A\}.$$

Consider the problem

$$\max \{z^T x : x \in C_A\} = \max \{z^T x : 1 - \langle h_i, x \rangle = \langle A_i, y \rangle \text{ for } i = 1, \dots, q, y \in S_+^k\}.$$

Strong duality holds since $\max \{z^T x : x \in C_A\}$ is a convex optimization problem and C_A has an interior point because it contains P . The dual program is given by

$$\min \{w^T \mathbf{1} : z = w^T H, w^T A \in S_+^k\}.$$

This gives

$$(C_A)^\circ = \{w^T H : w^T \mathbf{1} \leq 1, w^T A \in S_+^k\}. \tag{4.1}$$

□

Remark 4.3. We can replace the inequality $w^T \mathbf{1} \leq 1$ in (4.1) by the equality $w^T \mathbf{1} = 1$.

Proof. This proof is essentially the same as for [6, Remark 2.9]. There exists $s \geq 0$ such that $w^T \mathbf{1} + s = 1$. Since the polytopes P and Q contain 0 in their interiors, also the dual polytopes P° and Q° contain 0 in their interiors. Hence there exist $\lambda_1, \dots, \lambda_q \geq 0$ such that $\sum \lambda_i = 1$ and $\sum \lambda_i h_i = 0$. Define $\tilde{w} = w + s\lambda$ where $\lambda = (\lambda_i)$. Then

$$\begin{aligned}\tilde{w}^T \mathbf{1} &= w^T \mathbf{1} + s\lambda^T \mathbf{1} = w^T \mathbf{1} + s = 1, \\ \tilde{w}^T A &= w^T A + s\lambda^T A \in S_+^k\end{aligned}$$

because $\lambda \geq 0$ and each component is in S_+^k and

$$\tilde{w}^T H = w^T H + s\lambda^T H = w^T H.$$

□

Hence the dual bodies of C_A and C_B are

$$\begin{aligned}(C_A)^\circ &= \{z^T H : z^T \mathbf{1} = 1, z^T A \in S_+^k\}, \\ (C_B)^\circ &= \{x \in \mathbb{R}^n : \exists y \in S_+^k \text{ s.t. } 1 - \langle x, v_j \rangle = \langle y, B_j \rangle\}.\end{aligned}$$

As before if $\text{rank}(A_i) = 1$, then h_i lies in the rank one locus of the spectrahedral shadow $(C_B)^\circ$. In the primal picture this means that the spectrahedral shadow C_B touches the polytope Q at a generic point (i.e. a matrix of rank $k - 1$) on the boundary.

Concluding the discussion so far, the geometric version of Conjecture 4.1 is the following.

Conjecture 4.4. A matrix $S_{P,Q}$ is on the boundary $\partial \mathcal{M}_{k+1,k}^{p \times q}$ if and only if the shadow C_A contains all vertices of P at rank one loci and the spectrahedral shadow C_B touches all facets of Q at rank $k - 1$ loci.

Since $C_B \subseteq C_A$, the boundaries of C_A and C_B intersect at the vertices of P and at the tangency points with Q . This motivates us to state the following stronger conjecture:

Conjecture 4.5. A matrix $S_{P,Q}$ is on the boundary $\partial \mathcal{M}_{k+1,k}^{p \times q}$ if and only if for all spectrahedral shadows C such that $P \subseteq C \subseteq Q$, the shadow C contains $k + 1$ vertices of P at rank one loci and touches $k + 1$ facets of Q at rank $k - 1$ loci.

Example 4.6. Psd rank 3 rank 4 setting corresponds to the geometric configuration where a 3-dimensional projective spectrahedral shadow of 3×3 matrices is nested between 3-dimensional polytopes. A detailed study of generic spectrahedral shadows can be found in [15]. In our case there are three different types of spectrahedral shadows:

1. 3-dimensional spectrahedron of 3×3 matrices. For an example see Figure 4a. Its rank 1 locus is 0-dimensional and rank 2 locus is 2-dimensional. In Figure 4a, the rank 1 locus consists of the four nodes. The algebraic boundary is given by the determinant and has degree 3.
2. 3-dimensional projection of 4-dimensional spectrahedron of 3×3 matrices. The algebraic boundary of a generic spectrahedral shadow is irreducible of degree 6. This example is studied in detail in [14, Example 3.2] and depicted in [14, Figure 2].

3. 3-dimensional projection of 5-dimensional spectrahedron of 3×3 matrices. An example is the convex hull of the body depicted in Figure 4b. Both the rank 1 and rank 2 loci are degree 4 surfaces. Figure 4b depicts the rank 1 surface, the rank 2 surface consists of four linear planes.

A geometric configuration as in Conjecture 4.5 would be the following: The vertices of the interior polytope coincide with the nodes of the spectrahedron in Figure 4a and the facets of the outer polytope touch the boundary of this spectrahedron at rank 2 loci. In the dual picture, the vertices of the inner polytope lie on the rank 1 locus depicted in Figure 4b and the facets of the outer polytope contain the rank 2 locus of this spectrahedral shadow.

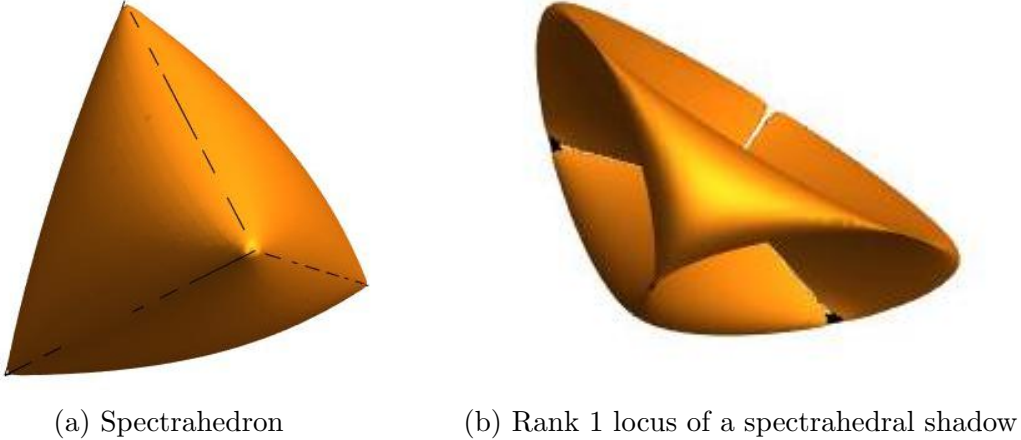


Figure 4: 3-dimensional spectrahedral shadows

We end this section with a restatement of the conjecture using Hadamard square roots.

Definition 4.7. Given a nonnegative matrix M , let \sqrt{M} denote a Hadamard square root of M obtained by replacing each entry in M by one of its two possible square roots. The square root rank of a nonnegative matrix M , denoted as $\text{rank}_{\sqrt{}}(M)$, is the minimum rank of a Hadamard square root of M .

Remark 4.8. Conjecture 4.1 is equivalent to the statement that a matrix $M \in \mathcal{M}_{k+1,k}^{(k+1) \times (k+1)}$ lies on the boundary $\partial \mathcal{M}_{k+1,k}^{(k+1) \times (k+1)}$ if and only if its square root rank is at most k . For example, in Figure 2b the set of matrices of square root rank at most two is defined by the vanishing locus of the boundary polynomial.

We conclude this section with a conjecture which would lead to a semialgebraic description of $\mathcal{M}_{k+1,k}^{(k+1) \times (k+1)}$.

Conjecture 4.9. Every matrix $M \in \mathcal{M}_{k+1,k}^{(k+1) \times (k+1)}$ has a psd factorization with at least $2k+1$ of the matrices in the factorization being rank 1.

5 Matrices of higher psd rank

In this section, we present partial results towards proving Conjecture 4.1.

5.1 Nested spectrahedra

We know from Theorem 2.1 that a matrix M has psd rank k if and only if it can fit a spectrahedral shadow coming from \mathcal{S}_+^k in between the two polytopes corresponding to M . In the following lemma, we show that M has psd rank k if and only if we can fit a spectrahedron in between P and Q . We do this by showing that if we have a spectrahedral shadow C such that $P \subseteq C \subseteq Q$, then we can find a spectrahedron C' such that $P \subseteq C' \subseteq C \subseteq Q$.

Lemma 5.1. *Let $M \in \mathbb{R}_{\geq 0}^{(k+1) \times (k+1)}$ be a full-rank matrix. Then, M has psd rank at most k if and only if one can nest a slice of the $k \times k$ psd cone (with no projections) between the two polytopes P and Q corresponding to M .*

Proof. If we can fit a slice of the $k \times k$ psd cone between the polytopes corresponding to M , then, M has psd rank at most k .

Now, suppose that M has psd rank at most k . Since M is full rank, we can factor it as $M = AB$, where $A, B \in \mathbb{R}^{(k+1) \times (k+1)}$ such that

$$A = \begin{pmatrix} 1 & 0 & \cdots & 0 & 1 \\ 0 & 1 & \cdots & 0 & 1 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1 & 1 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix} \quad \text{and} \quad B = A^{-1}M.$$

Then, the inner polytope P comes from a slice of the cone over the convex hull of the rows of A . Let the slice be given by last coordinate equal to 1. Then, P is the standard simplex in \mathbb{R}^k , i.e.

$$P = \text{conv}\{e_1, \dots, e_k, 0\}.$$

Since M has psd rank k , then there exists a slice of L of \mathcal{S}_+^k and a linear map π such that $C = \pi(L \cap \mathcal{S}_+^k)$ lies between P and Q :

$$P \subseteq C \subseteq Q.$$

If π is a $1 : 1$ linear map, then, the image C is just a linear transformation of a slice of \mathcal{S}_+^k , which is considered to be a slice. So, assume that π is not $1 : 1$, i.e. it has a kernel.

We can write

$$L \cap \mathcal{S}_+^k = \{(x_1, \dots, x_s) \mid \sum_{i=1}^s x_i A_i + (1 - \sum_i x_i) A_{s+1} \succeq 0\}$$

for some symmetric matrices A_1, \dots, A_{s+1} . Now, let u_1, \dots, u_s be an orthonormal basis of \mathbb{R}^s such that $\ker(\pi) = \text{span}(u_{k+1}, \dots, u_s)$. Let U be the orthogonal matrix with columns u_1, \dots, u_s . Consider new coordinates y such that $x = Uy$. Then, we can rewrite (after a transformation)

$$L \cap \mathcal{S}_+^k = \{(y_1, \dots, y_s) \mid \sum_i y_i B_i + (1 - (\sum_i y_i)) B_{s+1} \succeq 0\},$$

where B_1, \dots, B_{s+1} are linear combinations of the A_i 's. Then,

$$C = \{(y_1, \dots, y_k) | \exists y_{k+1}, \dots, y_s \text{ s.t. } \sum_i y_i B_i + (1 - (\sum_i y_i)) B_{s+1} \succeq 0\}.$$

We know that $P \subseteq C$ and $P = \text{conv}(e_1, \dots, e_k, 0)$. Since $e_i \in P \subseteq C$, then there exist $y_{k+1}^{(i)}, \dots, y_s^{(i)} \in \mathbb{R}$ such that

$$D_i := B_i + \sum_{j=k+1}^s [y_j^{(i)} (B_j - B_{s+1})] \succeq 0.$$

Since $0 \in P \subseteq C$, then, there exist $y_{k+1}^{(0)}, \dots, y_s^{(0)} \in \mathbb{R}$ such that

$$D_{k+1} := B_{s+1} + \sum_{j=k+1}^s [y_j^{(0)} (B_j - B_{s+1})] \succeq 0.$$

Consider the spectrahedron

$$C' := \{(y_1, \dots, y_k) | \sum_{i=1}^k y_i D_i + (1 - \sum_i y_i) D_{k+1} \succeq 0\}.$$

Note that $e_i \in C'$ for every $i = 1, \dots, k$ since $D_i \succeq 0$. Moreover, $0 \in C'$ since $D_{k+1} \succeq 0$. Thus, $P \subseteq C'$.

Moreover, if $(y_1, \dots, y_k) \in C'$, then

$$\begin{aligned} 0 &\preceq \sum_{i=1}^k y_i D_i + (1 - \sum_i y_i) D_{k+1} = \sum_{i=1}^k y_i (B_i + \sum_{j=k+1}^s [y_j^{(i)} (B_j - B_{s+1})]) \\ &\quad + (1 - \sum_i y_i) (B_{s+1} + \sum_{j=k+1}^s [y_j^{(0)} (B_j - B_{s+1})]) \\ &= \sum_{i=1}^k y_i B_i + \sum_{j=k+1}^s (\sum_{i=1}^k y_i y_j^{(i)} - (1 - \sum_{i=1}^k y_i) y_j^{(0)}) B_j \\ &\quad + (1 - \sum_{i=1}^k y_i - \sum_{j=k+1}^s (\sum_{i=1}^k y_i y_j^{(i)} - (1 - \sum_{i=1}^k y_i) y_j^{(0)})) B_{s+1}. \end{aligned}$$

Therefore, $(y_1, \dots, y_k) \in C$ and so $P \subseteq C' \subseteq C \subseteq Q$. Therefore, we can nest the spectrahedron C' in between P and Q . \square

Conjecture 5.2. *Lemma 5.1 holds for matrices of any size.*

Three different versions of nonnegative matrix factorizations appear in the literature: In [18] Vavasis considered the exact nonnegative factorization which asks whether a nonnegative matrix M has rank size nonnegative factorization. The geometric version of this question asks whether one can nest a simplex between the polytopes P and Q .

In [4] Gillis and Glineur defined restricted nonnegative rank as the minimum value r such that there exist $U \in \mathbb{R}_+^{p \times r}$ and $V \in \mathbb{R}_+^{r \times q}$ with $M = UV$ and $\text{rank}(U) = \text{rank}(V) = r$. The geometric interpretation of the restricted nonnegative rank asks for the minimal r such that there exist r points whose convex hull can be nested between P and Q .

The geometric version of the nonnegative rank factorization as defined in the introduction asks for the minimal r such that there exist r points whose convex hull can be nested between an $(r - 1)$ -dimensional polytope inside an q -simplex. These polytopes are not P and Q as defined in this paper. See [1, Theorem 3.1] for details.

In the positive semidefinite rank case there is no distinction between the psd rank and restricted psd rank, because taking an intersection with a subspace does not change the matrix size of a spectrahedral shadow while intersecting a polytope with a subspace can change the number of vertices. Conjecture 5.2 also suggests that there is no distinction between the spectrahedron and spectrahedral shadow case which we can compare with simplices and polytopes in the nonnegative rank case, or equivalently the exact nonnegative matrix factorization and restricted nonnegative factorization case.

We now show that given a spectrahedron C coming from \mathcal{S}_+^k such that $P \subseteq C \subseteq Q$, where P is a simplex and k of the vertices of P are also vertices of C , one can find a new spectrahedron C' such that $P \subseteq C' \subseteq C \subseteq Q$ such that all $k + 1$ of the vertices of P are also vertices of C' (in other words, they correspond to rank 1 matrices in C').

Lemma 5.3. *Let $P \subseteq \mathbb{R}^k$ be the simplex $P = \text{conv}(e_1, \dots, e_k, 0)$. Let C be a slice of \mathcal{S}_+^k such that $P \subseteq C$ and the vertices e_1, \dots, e_k correspond to rank one matrices. Then, we can find a slice C' of \mathcal{S}_+^k such that $P \subseteq C' \subseteq C$ with all $k + 1$ vertices of P corresponding to rank 1 matrices in C' .*

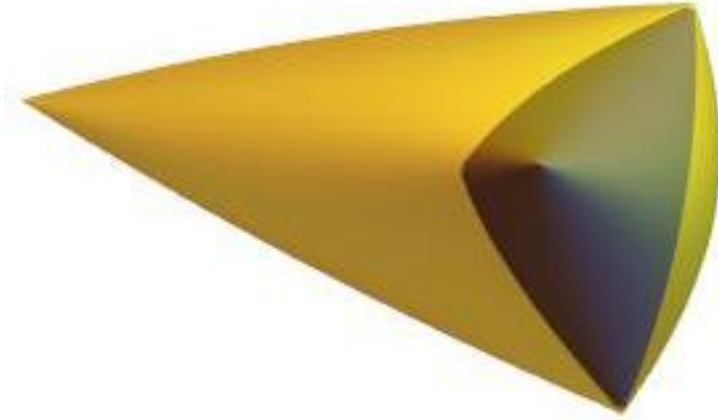


Figure 5: The spectrahedra C (in yellow) and C' (in blue) as in Lemma 5.3

Proof. This Lemma is trivial when $k = 1$. We proceed by induction.

By the conditions in the statement of the lemma, we can assume that

$$C = \{(x_1, \dots, x_k) | x_1 a_1 a_1^T + x_2 a_2 a_2^T + \dots + x_k a_k a_k^T + (1 - \sum_i x_i) B \succeq 0\},$$

where $B \succeq 0$ since $0 \in C$ and $a_1, \dots, a_k \in \mathbb{R}^k$ are vectors.

Suppose first that $\dim \text{span}\{a_1, \dots, a_k\} = \ell < k$. Let U be a change of coordinates that transforms $\text{span}\{a_1, \dots, a_k\}$ into $\text{span}\{e_1, \dots, e_\ell\}$. Then, if $a'_i = Ua_i$, we have that

$$C = \{(x_1, \dots, x_k) | x_1 a'_1 (a'_1)^T + x_2 a'_2 (a'_2)^T + \dots + x_k a'_k (a'_k)^T + (1 - \sum_i x_i) U B U^T \succeq 0\},$$

where $B' := U B U^T$ is still positive semidefinite. If $B'_{i,j} = 0$ for all $i, j \geq \ell + 1$, then, the statement reduces to the case of ℓ , which is true by induction. So, suppose that, say, (since $B' \succeq 0$) $B'_{\ell+1, \ell+1} > 0$. Then, choose a vector $d \in \mathbb{R}^k$ such that $d_{\ell+1} \neq 0$ and $dd^T \preceq B'$. Consider the spectrahedron

$$C' := \{(x_1, \dots, x_k) | x_1 a'_1 (a'_1)^T + x_2 a'_2 (a'_2)^T + \dots + x_k a'_k (a'_k)^T + (1 - \sum_i x_i) dd^T \succeq 0\}.$$

First note that clearly $e_1, \dots, e_k, 0 \in C'$. We will show that $C' \subseteq C$. Indeed, let $(x_1, \dots, x_k) \in C'$. Since $(a'_i)_{\ell+1} = 0$ for all i , $d_{\ell+1} \neq 0$ and

$$x_1 a'_1 (a'_1)^T + x_2 a'_2 (a'_2)^T + \dots + x_k a'_k (a'_k)^T + (1 - \sum_i x_i) dd^T \succeq 0,$$

we have $(1 - \sum_i x_i) \geq 0$. But then

$$\begin{aligned} 0 &\preceq x_1 a'_1 (a'_1)^T + x_2 a'_2 (a'_2)^T + \dots + x_k a'_k (a'_k)^T + (1 - \sum_i x_i) dd^T \\ &\preceq x_1 a'_1 (a'_1)^T + x_2 a'_2 (a'_2)^T + \dots + x_k a'_k (a'_k)^T + (1 - \sum_i x_i) B' \end{aligned}$$

and, therefore, $C' \subseteq C$.

Now, assume that $\dim \text{span}\{a_1, \dots, a_k\} = k$. Then, let U be an invertible transformation such that $Ua_i = e_i$. Then,

$$C = \{(x_1, \dots, x_k) | x_1 e_1 e_1^T + x_2 e_2 e_2^T + \dots + x_k e_k e_k^T + (1 - \sum_i x_i) U B U^T \succeq 0\},$$

where $B' := U B U^T \succeq 0$. Let $d \in \mathbb{R}^k$ be such that $d_i = \sqrt{B'_{i,i}}$ and let $S \in \mathbb{R}^{k \times k}$ be such that

$$S_{i,j} = \begin{cases} \frac{B'_{i,j}}{\sqrt{B'_{i,i} B'_{j,j}}} & \text{if } B'_{i,i} B'_{j,j} \neq 0, \\ 1 & \text{if } B'_{i,i} B'_{j,j} = 0 \text{ and } i = j, \\ 0 & \text{if } B'_{i,i} B'_{j,j} = 0 \text{ and } i \neq j. \end{cases}$$

Since $B' \succeq 0$, it is clear that $S \succeq 0$ as well since it is obtained from B' by rescaling some rows and columns and by adding 1 on the diagonal in places that are 0 in B' . Let

$$C' = \{(x_1, \dots, x_k) | x_1 e_1 e_1^T + x_2 e_2 e_2^T + \dots + x_k e_k e_k^T + (1 - \sum_i x_i) dd^T \succeq 0\}.$$

Then, clearly $e_1, \dots, e_k, 0 \in C'$. We will show that $C' \subseteq C$. Let $(x_1, \dots, x_k) \in C'$. Then,

$$x_1 e_1 e_1^T + x_2 e_2 e_2^T + \dots + x_k e_k e_k^T + (1 - \sum_i x_i) d d^T \succeq 0. \quad (5.1)$$

By the Schur Product Theorem, we know that the Hadamard product of two positive semidefinite matrices is positive semidefinite. Therefore, when we take the Hadamard product of the matrix (5.1) with S we get a positive semidefinite matrix. But that Hadamard product equals

$$x_1 e_1 e_1^T + x_2 e_2 e_2^T + \dots + x_k e_k e_k^T + (1 - \sum_i x_i) B' \succeq 0,$$

therefore, $C' \subseteq C$. □

5.2 Computational results

In this section we provide computational evidence for Conjecture 4.1 when $k > 2$.

Example 5.4. We consider the 2-dimensional family of 4×4 circulant matrices

$$\begin{bmatrix} a & b & 1 & b \\ b & a & b & 1 \\ 1 & b & a & b \\ b & 1 & b & a \end{bmatrix} \quad (5.2)$$

which is parametrized by a and b .

In Figure 6, the 4126 green dots correspond to randomly chosen matrices of the form (5.2) that have psd rank at most three. The psd rank is computed using the code provided by the authors of [17] adapted to the computation of the semidefinite rank [10, Section 5.6]. The red curves correspond to matrices of the form (5.2) that have a psd factorization by 3×3 rank one matrices. These curves are obtained by an elimination procedure in Macaulay2.

Example 5.5. We construct $k \times k$ positive semidefinite matrices $A_1, \dots, A_p, B_1, \dots, B_q$ of ranks r_1, \dots, r_{p+q} . We construct a matrix M such that $M_{ij} = \langle A_i, B_j \rangle$. We vectorize the matrix M and compute its Jacobian J with respect to the entries of $A_1, \dots, A_p, B_1, \dots, B_q$. Finally we substitute the entries of $A_1, \dots, A_p, B_1, \dots, B_q$ by random nonnegative integers and compute the rank of J . If $\text{rank}(J) = pq - 1$, then matrices that have psd factorization by $\{r_1, \dots, r_p\}, \{r_{p+1}, \dots, r_{p+q}\}$ rank matrices give a candidate for a boundary component.

The possible candidates for $k = 3$ are summarized in Table 1. For all p, q the case where four matrices A_i and four matrices B_j have rank 1 and all other matrices have any rank greater than 1 are represented. For $k = 4$ the analogous statement is not true. If $M \in \mathbb{R}^{10 \times 10}$, exactly five A_i and five B_j matrices have rank one and the rest of the matrices have rank two, then the Jacobian has rank 94. If the rest of the matrices in the psd factorization have rank three or four, then the Jacobian has rank 99 as expected. Hence without further constraints on the ranks of the rest of the matrices Conjecture 4.1 does not hold for general r and k .

Example 5.6. Using the same strategy as in Example 5.5, we have checked that the Jacobian has expected dimension for $r = k + 1$ and $k < 10$.

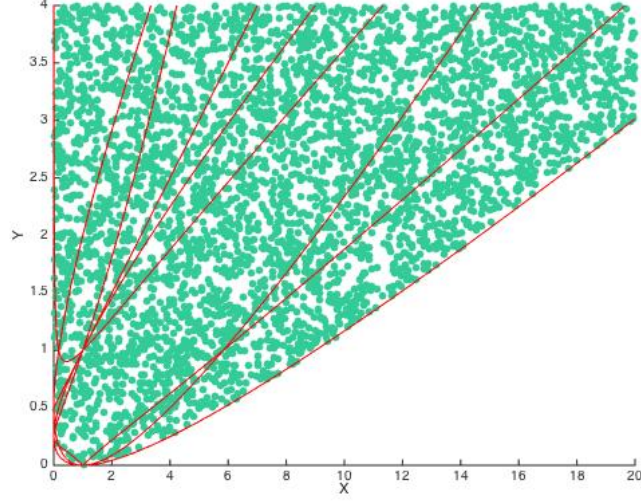


Figure 6: A family of 4×4 circulant matrices of psd rank at most 3

psd rank	p	q	ranks
3	4	4	$\{\{1,1,1,1\}, \{1,1,1,1\}\}$
3	4	5	$\{\{1,1,1,1\}, \{1,1,1,1,2/3\}\}$
3	4	6	$\{\{1,1,1,1\}, \{1,1,1,1,2/3,2/3\}\}, \{\{1,1,1,2\}, \{1,1,1,1,1,1\}\}$
3	5	5	$\{\{1,1,1,1,2/3\}, \{1,1,1,1,2/3\}\}$
3	5	6	$\{\{1,1,1,1,2/3\}, \{1,1,1,1,2/3,2/3\}\}, \{\{1,1,1,2,3\}, \{1,1,1,1,1,1\}\}$
3	6	6	$\{\{1,1,1,1,2/3,2/3\}, \{1,1,1,1,2/3,2/3\}\}, \{\{1,1,1,1,1,1\}, \{1,1,1,2,3,3\}\},$ $\{\{1,1,1,1,1,1\}, \{1,1,2,2,2,2\}\}, \{\{1,1,1,1,1,2\}, \{1,1,1,2,2,2\}\}$

Table 1: Ranks of matrices in the psd factorization of a psd rank three matrix that can potentially give boundary components

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